

WHAT IS CLAIMED IS:

1. A negative electrode material for a non-aqueous electrolyte secondary battery capable of reversibly absorbing and desorbing lithium,
5 comprising a solid phase A and a solid phase B that have different compositions; and
having a structure in which a surface around the solid phase A is entirely or partly covered by the solid phase B,
wherein the solid phase A contains at least one element selected from
10 the group consisting of silicon, tin and zinc,
the solid phase B contains said at least one element, and at least one element selected from the group consisting of Group IIA elements, transition elements, Group IIB elements, Group IIIB elements and Group IVB elements, and
15 the solid phase A is in at least one state selected from the group consisting of an amorphous state and a low crystalline state.
2. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 1,
20 wherein no peak attributed to a crystal plane of the solid phase A is present on a diffraction line obtained by a wide angle X-ray diffraction measurement (X-ray diffraction measurement in a range of a diffraction angle 2θ of 10° to 80° , when using $\text{CuK}\alpha$ radiation as an X-ray source).
- 25 3. A negative electrode material for a non-aqueous electrolyte secondary battery capable of reversibly absorbing and desorbing lithium,
comprising a solid phase A and a solid phase B that have different compositions; and
having a structure in which a surface around the solid phase A is
30 entirely or partly covered by the solid phase B,
wherein the solid phase A contains at least one element selected from the group consisting of silicon, tin and zinc,
the solid phase B contains said at least one element, and at least one
element selected from the group consisting of Group IIA elements, transition
35 elements, Group IIB elements, Group IIIB elements and Group IVB elements, and
a crystallite size of the solid phase A is in the range of at least 5 nm

and at most 100 nm.

4. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 1,

5 wherein the solid phase A is a solid phase in at least one state selected from the group consisting of an amorphous state and a low crystalline state, even after a heat treatment at 100°C or higher.

5. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 1,

10 wherein the solid phase A is a solid phase in which a crystallite size of the solid phase A is in the range of at least 5 nm and at most 100 nm, when a heat treatment at 100°C or higher is performed.

6. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 3,

15 wherein the solid phase A is a solid phase in which a crystallite size of the solid phase A is in the range of at least 5 nm and at most 100 nm, when a heat treatment at 100°C or higher is performed.

20 7. A negative electrode material for a non-aqueous electrolyte secondary battery capable of reversibly absorbing and desorbing lithium, comprising a solid phase A and a solid phase B that have different compositions; and

25 having a structure in which a surface around the solid phase A is entirely or partly covered by the solid phase B,

wherein the solid phase A contains at least one element selected from the group consisting of silicon, tin and zinc,

30 the solid phase B contains said at least one element, and at least one element selected from the group consisting of Group IIA elements, transition elements, Group IIB elements, Group IIIB elements and Group IVB elements,

the solid phase A contains a first crystal structure, and

35 the solid phase B contains a second crystal structure represented by a space group differing from the space group that represents the first crystal structure.

8. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 7,
wherein a ratio of the second crystal structure in the solid phase B is in the range of at least 60 wt% and at most 95 wt%.
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9. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 7,
wherein the second crystal structure in the solid phase B contains a crystal structure represented by at least one selected from the group consisting of space group C and space group F, where the space group C and the space group F are space groups in Bravais lattice notation.
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10. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 9,
wherein the second crystal structure in the solid phase B contains a crystal structure represented by the space group Cmcm as annotated by Hermann-Mauguin symbols.
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11. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 1,
wherein a weight ratio of the solid phase A is in the range of at least 5 wt% and at most 40 wt% and a weight ratio of the solid phase B is in the range of at least 60 wt% and at most 95 wt% in the negative electrode material.
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12. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 3,
wherein a weight ratio of the solid phase A is in the range of at least 5 wt% and at most 40 wt% and a weight ratio of the solid phase B is in the range of at least 60 wt% and at most 95 wt% in the negative electrode material.
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13. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 7,
wherein a weight ratio of the solid phase A is in the range of at least 5 wt% and at most 40 wt% and a weight ratio of the solid phase B is in the range of at least 60 wt% and at most 95 wt% in the negative electrode material.
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material.

14. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 1,

5 wherein the solid phase A comprises Si and the solid phase B comprises Ti and Si.

15. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 14,

10 wherein the solid phase B contains TiSi_2 .

16. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 15,

15 wherein the TiSi_2 comprises a crystal structure represented by the space group Cmc \bar{m} as annotated by Hermann-Mauguin symbols.

17. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 15,

20 wherein the solid phase B contains an amorphous body of at least one element selected from the group consisting of Ti and Si.

18. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 3,

25 wherein the solid phase A comprises Si and the solid phase B comprises Ti and Si.

19. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 18,

30 wherein the solid phase B contains TiSi_2 .

20. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 19,

35 wherein the TiSi_2 comprises a crystal structure represented by the space group Cmc \bar{m} as annotated by Hermann-Mauguin symbols.

21. The negative electrode material for a non-aqueous electrolyte secondary battery according to claim 19,

wherein the solid phase B contains an amorphous body of at least one element selected from the group consisting of Ti and Si.

22. The negative electrode material for a non-aqueous electrolyte
5 secondary battery according to claim 7,
wherein the solid phase A comprises Si and the solid phase B
comprises Ti and Si.

23. The negative electrode material for a non-aqueous electrolyte
10 secondary battery according to claim 22,
wherein the solid phase B contains TiSi_2 .

24. The negative electrode material for a non-aqueous electrolyte
secondary battery according to claim 23,
15 wherein the TiSi_2 comprises a crystal structure represented by the
space group Cmc21 as annotated by Hermann-Mauguin symbols.

25. The negative electrode material for a non-aqueous electrolyte
secondary battery according to claim 23,
20 wherein the solid phase B contains an amorphous body of at least one
element selected from the group consisting of Ti and Si.

26. A non-aqueous electrolyte secondary battery comprising:
a negative electrode containing the negative electrode material for a
25 non-aqueous electrolyte secondary battery according to claim 1;
a positive electrode capable of reversibly absorbing and desorbing
lithium; and
a non-aqueous electrolyte having lithium ion conductivity.

30 27. A non-aqueous electrolyte secondary battery comprising:
a negative electrode containing the negative electrode material for a
non-aqueous electrolyte secondary battery according to claim 3;
a positive electrode capable of reversibly absorbing and desorbing
lithium; and
35 a non-aqueous electrolyte having lithium ion conductivity.

28. A non-aqueous electrolyte secondary battery comprising:

a negative electrode containing the negative electrode material for a non-aqueous electrolyte secondary battery according to claim 7;

a positive electrode capable of reversibly absorbing and desorbing lithium; and

5 a non-aqueous electrolyte having lithium ion conductivity.

29. A method for producing a negative electrode material for a non-aqueous electrolyte secondary battery, comprising:

10 a first step of mixing a material containing at least one element selected from the group consisting of silicon, tin and zinc with a material containing at least one element selected from the group consisting of Group IIA elements, transition elements, Group IIB elements, Group IIIB elements and Group IVB elements, and melting the resulting material;

15 a second step of forming a solidified material by quenching and solidifying the melted material; and

a third step of obtaining a powder comprising a solid phase A and a solid phase B that have different compositions and having a structure in which a surface around the solid phase A is entirely or partly covered by the solid phase B, by performing a mechanical alloying process on the solidified material.

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30. The method for producing a negative electrode material for a non-aqueous electrolyte secondary battery according to claim 29, further comprising a step of heat treating the powder, after the third step.

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